ABSTRACT

This invention provides a method for predicting pharmacokinetic properties of molecules comprising the steps of:

(a) preparing 2D-structures of molecules used as a training set;

(b) constructing a 2D-fingerprint by counting the number of structural descriptors that potentially relate to a pharmacokinetic property, either manually or automatically using internally developed macro; wherein said structural descriptors consist of predefined 20 to 80 atoms/fragments or substructures;

(c) analyzing the obtained 2D-fingerprint by a statistical analysis method to correlate with the pharmacokinetic property of the molecule to yield a quantitative structure-property relationship (QSPR) model; and

(d) calculating the pharmacokinetic property of a trial molecule using the above obtained QSPR model.

A system for this invention is also provided. According to this method and system, it is possible to predict pharmacokinetic properties of molecules prior to synthesis, without labor-intensive and time-consuming experimentation.